Suspect Screening and Non-Targeted Analysis of Drinking Water Using Point-Of-Use Filters

Supporting Information

Text and Figures

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Materials

Dichloromethane (DCM) and methanol (B&J Brand High Purity Solvent) were purchased from Honeywell Burdick & Jackson (Muskegon, MI, USA). Ammonium acetate and ammonium formate were purchased from Sigma Aldrich (St. Louis, MO, USA). Ultrapure deionized (DI) water was generated in house from a Barnsted Easypure UV/UF (Dubuque, IA, USA) coupled with activated charcoal and ion exchange resin canisters.

Figure S1 - Bubble plot of all features found in the Brita® extract colored by positive and negative ionization mode, and whether they were matched or unmatched to a formula in the database. The size of the bubble is proportional to the size of its corresponding chromatographic peak.

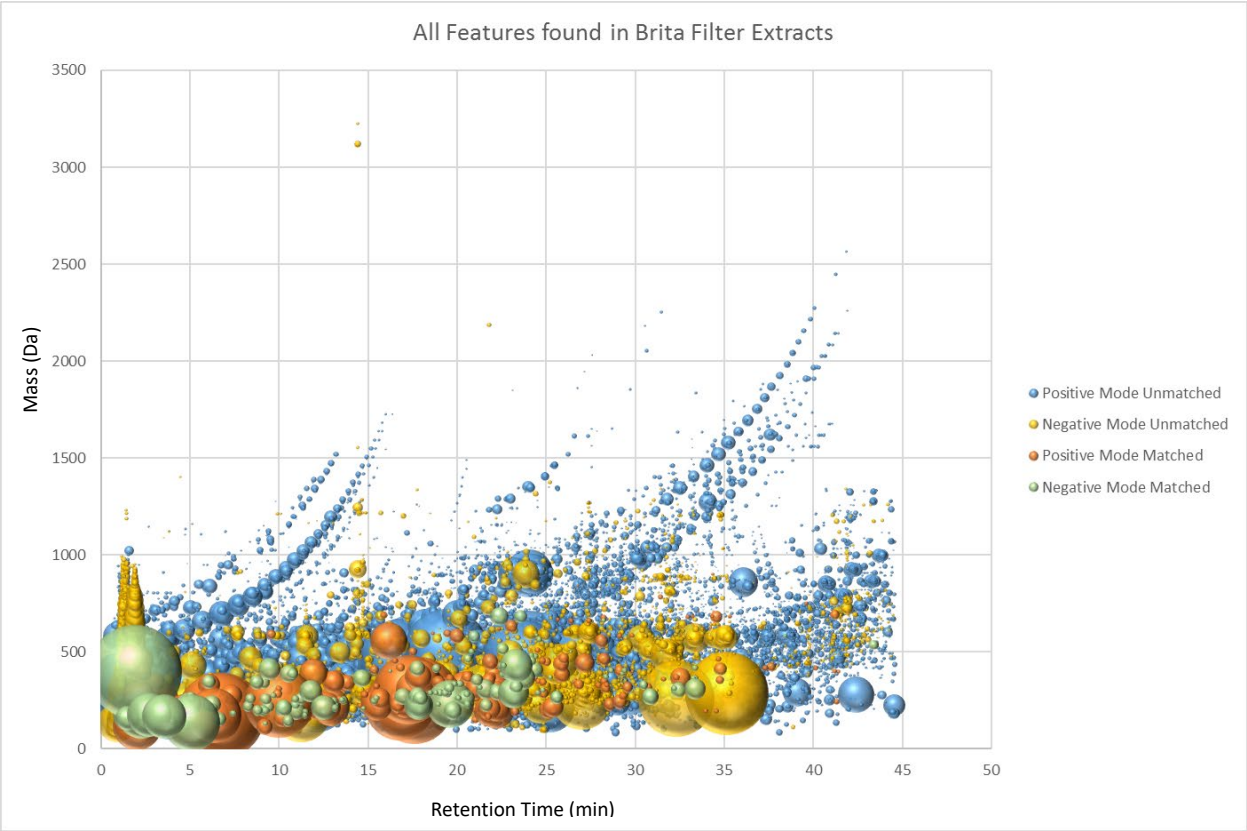

Figure S2 – PCA using the parsed formulas from the water filters and house dust samples from Rager *et al.* C = carbon, Cl = chlorine, F = fluorine, H = hydrogen, N = nitrogen, O = oxygen, P = phosphorous, RT = retention time, S = sulfur. Bromine was omitted due to its lack of occurrence (one house dust formula and no Brita® formulas contained bromine).

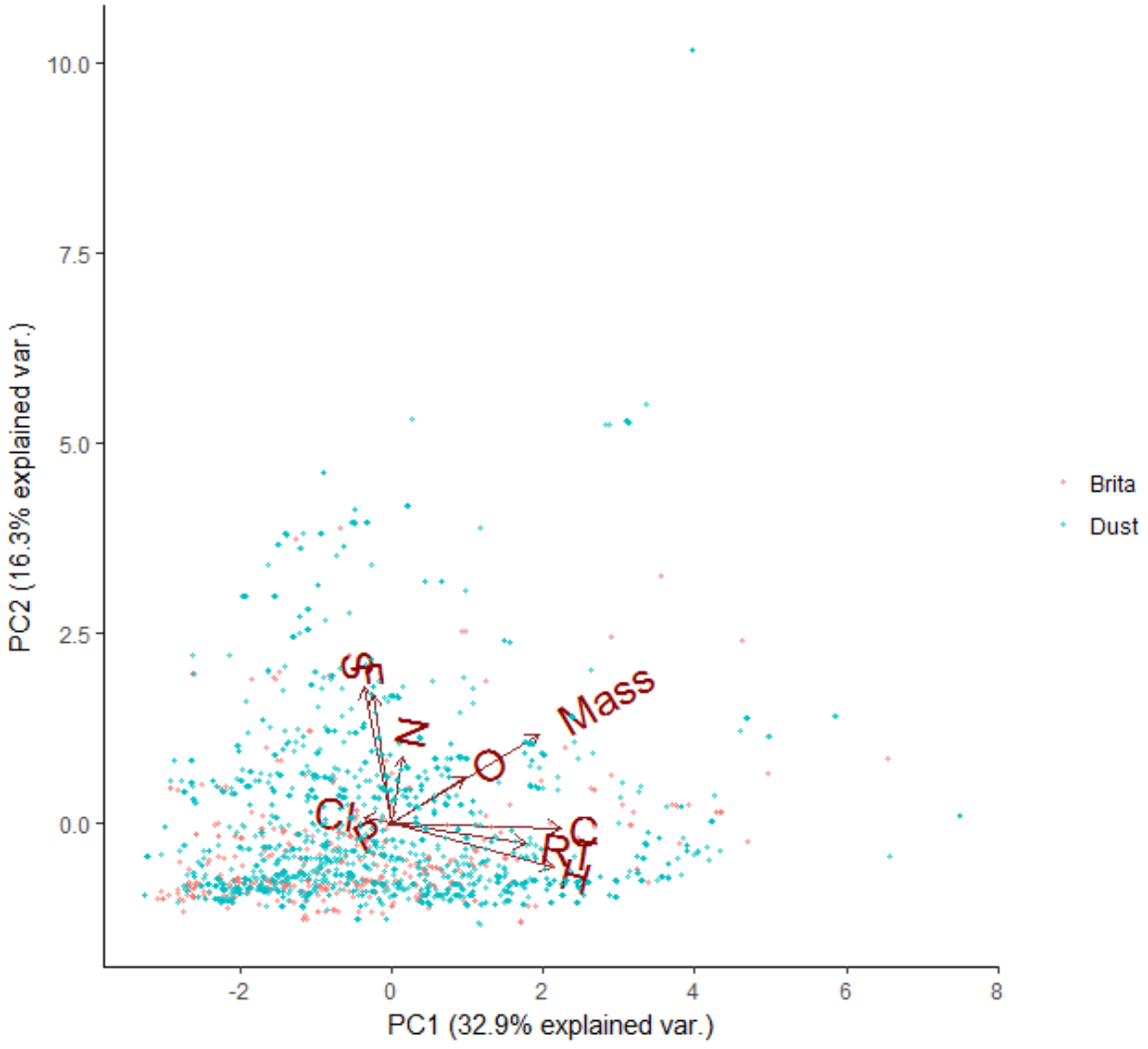

Figure S3 – Loadings plot from the PCA of product-use categories.

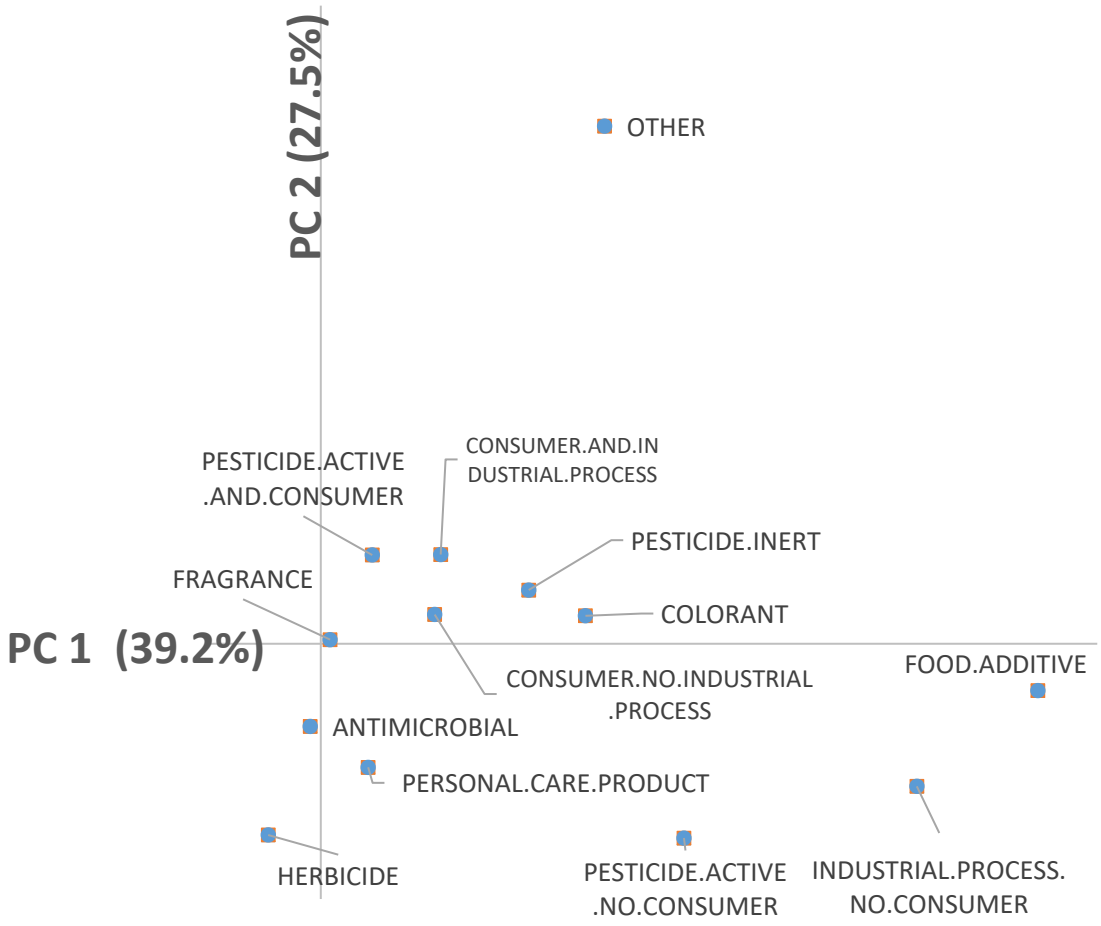

Figure S4 – A) Chromatograms of decarboxylated PFOA, B) Chromatogram of PFOA, and C) Spectrum of the two compounds showing the mass difference between the two (43.9901) corresponding to CO_2

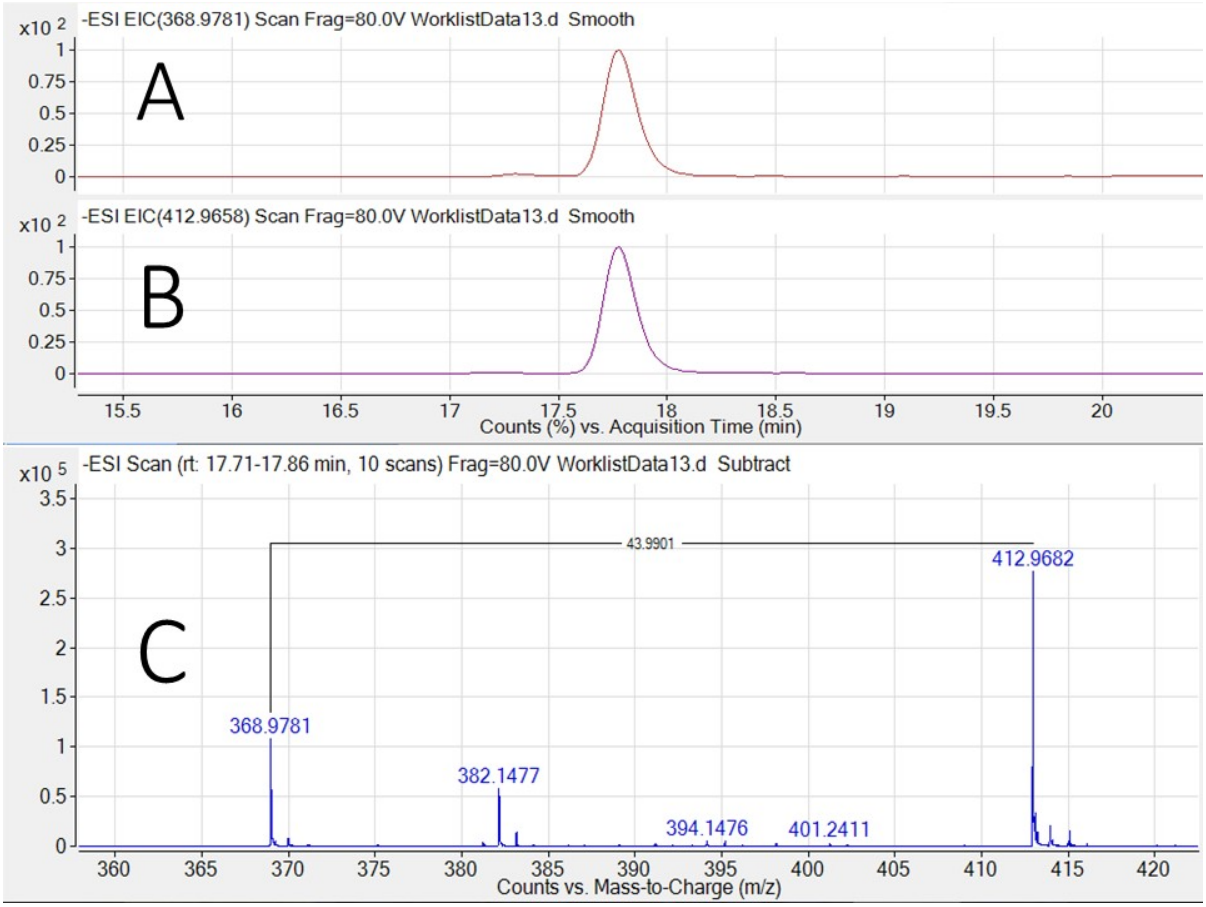

Figure S5 – Chromatograms of A) m/z 518.8796 unknown peak in Pittsboro Tap sample, B) m/z 564.8848 unknown peak in Pittsboro Tap sample, C) m/z 564.8848 unknown peak in a method blank, and D) blank subtracted spectrum at m/z 564.8848 in Pittsboro Tap sample with theoretical spectrum of the formula $C_{13}H_{22}C1_7O_7P$ ($C_{12}H_{20}Cl_7O_5P$ + formate adduct) in red boxes.